Partial quantum statistics and its implications for narrow band materials

T. Zhou*

Bell Laboratories, Lucent Technologies,

791 Holmdel Road, Holmdel, New Jersey 07733, U.S.A.

Abstract

Based upon the newly proposed partial quantum statistics [T. Zhou, Solid State Commun. **115**, 185 (2000)], some canonical physical properties of partially localized electron systems have been calculated. The calculated transport and superconducting properties of such systems are very different from those of Landau-Fermi liquids, but display some striking similarities to the properties of high temperature superconductors and some other narrow band materials.

PACS numbers: 71.28.+d, 05.90.+m, 72.10.-d, 74.25.-q

Bloch states are essentially unbound states. A Bloch wave function at any given time is nonzero in the whole crystal lattice except its nodal points. Because of their identical intrinsic properties and delocalized nature Bloch electrons are indistinguishable from each other. Neglecting their mutual interactions, a system consisting of Bloch electrons is thus an ideal Fermi gas system and strictly obeys the Fermi-Dirac (F.D.) statistics at any temperature, though at high temperature the Maxwell-Boltzmann (M.B.) distribution is a good approximation. On the other end of the spectrum, when electrons are localized and completely separated from each other like the electrons of magnetic ions in paramagnetic salts, these electrons are in bound states, and the wave function of one electron (or the many-body wave function of several electrons of the same ion) does not overlap with another spatially. These electrons thus become distinguishable, and the system strictly obeys the M.B. distribution at any temperature [1]. This is of course in consistent with the Langevin paramagnetic behavior observed in paramagnetic salts down to very low temperature [1, 2], and in contrast to the Pauli paramagnetism expected in Fermi gas systems. Bloch electrons, on the other hand, can be localized in real space by strong electron-electron interaction (large Hubbard U), strong electron-phonon interaction (*e.g.* small polaron), and/or by disorder (Anderson localization). In fact, paramagnetic salts with ions containing only one 3d or 4f electron (or hole) can be taken as an extreme and simple example where the Hubbard U is infinite and no site can be occupied by two electrons (or two holes) simultaneously. Now the question is, when the electrons are neither completely localized as in the paramagnetic salts, nor completely delocalized as the Bloch electrons, what kind of statistical distribution should they obey? Should the electrons, after their mutual interactions are taken into account by renormalization, always adopt the F.D. statistics as indicated in the Landau Fermi-liquid theorem?

In a gedanken experiment recently proposed by the author [3], it has been shown that in any self-consistent theory for partially localized electrons (PLE), neither the F.D. nor the M.B. distribution can be the right answer, and there has to be a partial Fermi (p.F.) statistics which is different from both the F.D. and M.B. statistics. Furthermore, it has been argued by the author that in order to reach such a p.F. statistics, the Slater-determinant type many-body wave function used to describe the Fermi gas system has to be modified, and the many-body wave function proposed by the author [3] violates the anti-symmetry requirement for the wave function of identical fermions. The particle exchange symmetry thus becomes

a broken symmetry, and it was argued in Ref. [3] that the breaking of such a symmetry in PLE systems does not violate any fundamental quantum mechanics principle, including Pauli's exclusion principle. The conventional belief that quantum field theory requires the wave function of identical fermions to be anti-symmetric is not applicable here. The reason is that quantum field theory always assumes, explicitly or implicitly, that identical particles are indistinguishable. This assumption is not true here because localized electrons can be distinguished. Based on this new form of wave function a parameter η, which is a real number between 0 and 1, is defined to describe the indistinguishable degree of PLE system [3]. When $\eta = 1$, the electrons are completely delocalized and indistinguishable; when $\eta = 0$, the electrons are completely localized and distinguishable. The p.F. statistical distribution is subsequently deduced to describe the PLE gas system. Suppose $f_{pF}(E_l, T)$ is the probable number of electrons with indistinguishable degree η occupying any state with an energy level E_l at temperature T, one then has [3]

$$f_{pF}(E_l, T) = \frac{1}{e^{(E_l-\mu)/k_BT} + \eta},$$
$$\sum_l \omega_l f_{pF}(E_l, T) = N. \tag{1}$$

Here k_B is the Boltzmann constant, ω_l is the degeneracy degree of the lth energy level, and the chemical potential μ is still determined by the total electron number N. It is evident from Eq. (1) that when $\eta = 1$ or 0, the F.D. or M.B. distribution is recovered, respectively [3]. We note that the exact mathematical form of Eq. (1) has appeared in Ref. [4] and [5], but there the physical contexts were very different.

It was proposed [3] that f_{pF} should have significant deviation from the F.D. or M.B distribution in narrow-band materials [6], since electrons are neither very delocalized nor very localized in these materials. In this letter, we will demonstrate that systems obeying the p.F. statistics have properties that are very different from those of Landau-Fermi liquids, but are strikingly similar to many properties of high temperature superconductors and some other narrow band materials.

We first examine Eq. (1), in which the summation of all states can be replaced by the integral $\int_0^\infty g(E) f_{pF}(E, T) dE = N$. Here $g(E)$ is the total density of states, which includes both the delocalized and localized components. $g(E)$ for a p.F. gas system is the same as a Fermi gas system with the same energy spectrum. The effective delocalization density of

states $g'(E)$ in a p.F. system with electron indistinguishable degree η, however, is only

$$g'(E) = \eta g(E), \tag{2}$$

according to the definition of η [3]. Replacing $g(E)$ by $g'(E)$, and rewriting Eq. (1) so that it is easier to compare it with the F.D. distribution, one reaches

$$f'_{pF}(E,T) = \frac{\eta^{-1}}{e^{[E-(E_{pF}+k_BT\ln\eta)]/k_BT}+1},$$
$$\int_0^\infty g'(E) f'_{pF}(E,T)dE = N. \tag{3}$$

Here $f'_{pF}(E,T)$ is the distribution function for the delocalization component of a p.F. gas system. The chemical potential μ is replaced by E_{pF}, the effective Fermi energy in a p.F. system for the delocalization component, and we call it partial Fermi energy. Assuming that a Fermi gas system with Fermi energy E_F has the same $g(E)$ as the p.F. gas system in discussion, and E_F^0 is the Fermi energy at $T=0$, solving Eq. (3) one has $E_{pF}(T=0) = E_F^0$, and $f'_{pF}(T=0) = \eta^{-1}$ or 0 for $E <$ or $> E_F^0$, respectively. At $T > 0$ but $k_BT \ll E_F^0$, solving Eq. (3) again and we find that to the first order approximation of T,

$$E_{pF}(T) \approx E_F^0 + k_BT\ln\eta^{-1}. \tag{4}$$

Here we have assumed that $g(E)$ is a smooth function near E_F^0. Combining Eqs. (3) and (4) one reaches

$$f'_{pF}(E,T) \approx \frac{\eta^{-1}}{e^{(E-E_F^0)/k_BT}+1} \approx \eta^{-1} f_F(E,T). \tag{5}$$

Here $f_F(E,T)$ is the F.D. distribution function. Approximating to the first order of T, $E_F(T) \approx E_F^0$ in a Fermi gas system [2]. We also note that in a p.F. system, if the spin degree of freedom can be ignored, then $g'(E)$, rather than $g(E)$, is the density of states that is mostly relevant to the observable physical properties. The schematic illustration of the p.F. and F.D. distributions at finite temperature is shown in Fig. 1.

Equations (2), (4), and (5) essentially summarize the differences between the Fermi statistics and the p.F. statistics at low temperature. In the following we will use these equations to calculate some canonical thermodynamic, transport and superconducting properties of p.F. systems. To compare these calculations with the physical properties of some real narrow band materials, we take cuprates as the prime examples [7, 8]. Undoped cuprates are

Mott-Hubbard insulators, which are extremely localized electron systems. The overdoped cuprates with doping concentration $x > 0.3$, however, are believed to be Fermi-liquid systems, and carriers in these materials are essentially Bloch type and delocalized. Carriers in cuprates with $0 < x < 0.3$ are believed to be between these two extreme cases and partially localized. Cuprates thus provide us a perfect set of real systems, whose physics is closely associated with the delocalization degree of the carriers. The discussion above led us to believe that the delocalization degree of carriers in cuprates can be quantified by η, and η should increase monotonically with the doping concentration x.

We first calculate the electronic specific heat, one of the most important thermodynamic properties, of a p.F. gas system. For a Fermi gas system the electronic specific heat C_{el} at temperature $k_BT \ll E_F$ is proportional to T with a linear coefficient $\gamma = \frac{1}{3}\pi^2 k_B^2 g(E_F)$ [2]. For a p.F. gas system, replacing $g(E)$ and $f_F(E,T)$ by Eqs. (2) and (5), respectively, one finds that at temperature $k_BT \ll E_{pF}$, C_{el} is the same as the Fermi gas system with the same total density of states $g(E)$. The reason is that the total energy of a Fermi or p.F. gas system is decided by $g(E)f_F(E,T)$ or $g'(E)f'_{pF}(E,T)$. Since these two products are equal according to Eqs. (2) and (5), C_{el}, the derivative of the total energy, should also be equal in these two systems. Experiments show that for optimally doped and overdoped cuprates, the normal state γ is indeed independent of temperature and doping concentration at least up to 300 K [9]. This is consistent with our calculation above of the p.F. gas system. In the underdoped regime, below a characteristic temperature T^* γ decreases with decreasing T, and this is believed to be related to the pseudogap [9]. Since our discussion above does not take into account any anomaly in $g'(E)$ such as a pseudogap, our calculation is thus not comparable with the experimental results in the underdoped cuprates. Other thermodynamic properties that are also decided by $g'(E)f'_{pF}(E,T)$ should yield similar results as C_{el}, and experiments show that the magnetic susceptibility data are indeed consistent with the C_{el} results in the optimally doped to overdoped regime [9].

We now turn to the calculation of transport properties. For Fermi-liquid metals, the dominant scattering mechanism at low temperature is electron-electron scattering, in which the total energy and momentum should be conserved while the Fermi statistics should also be obeyed. The Fermi statistics acts twice, each time reduces the scattering rate τ_{ee}^{-1} approximately by a factor of k_BT/E_F, or $\hbar\omega/E_F$ in the case of zero temperature low energy excitation with excitation energy $\hbar\omega$ [2]. Suppose τ_{cee}^{-1} is the classical electron-electron scattering

rate after taking into account the Coulomb screening effect but without the consideration of the Fermi statistics. The scattering rate after including the Fermi statistics then becomes $\tau_{ee}^{-1} \approx (k_B T/E_F)^2 \tau_{cee}^{-1}$ or $(\hbar\omega/E_F)^2 \tau_{cee}^{-1}$ [2]. To calculate τ_{ee}^{-1} in a p.F. system, one should replace the Fermi statistics by the p.F. statistics using Eq. (5). (τ_{ee}^{-1} as a function of T or ω is not dependent on the density of states). Equation (5), on the other hand, indicates that the restriction on the electron-electron scattering process imposed by the Fermi statistics is partially lifted in a p.F. system, with the parameter η^{-1} linearly interpolating between the Fermi statistics and the purely classical M.B. statistics where there is no statistical restriction at all. Therefore, one can express τ_{ee}^{-1} of a p.F. system as

$$\begin{aligned} \tau_{ee}^{-1} &\approx (k_B T/E_F^0)^{2\eta} \tau_{cee}^{-1} \quad or \\ \tau_{ee}^{-1} &\approx (\hbar\omega/E_F^0)^{2\eta} \tau_{cee}^{-1}. \end{aligned} \tag{6}$$

Note that E_F is replaced by E_F^0 here due to Eq. (5). For $\eta = 1$ or 0, the Fermi-liquid behavior or the classical behavior is recovered, respectively.

When $\eta = \frac{1}{2}$, one has $\tau_{ee}^{-1} \sim T$ *or* ω, which is the well known marginal Fermi-liquid (MFL) phenomenology formulated to describe optimally doped cuprates [10, 11]. As analyzed by the MFL theory [10, 11, 12], this linear T or ω dependence explains many transport properties of optimally doped cuprates, including an electronic Raman background which is both T and ω independent, an optical conductivity which decreases with ω like ω^{-1}, a dc resistivity ρ which has the celebrated linear T dependence, *etc.* With x increasing from the optimally doping value, η is expected to increase from $\frac{1}{2}$ to 1, as discussed above. Equation (6) thus also naturally explains the gradual crossover from the MFL behavior to Fermi-liquid behavior with increasing doping, which is best evidenced experimentally by ρ's gradual change from T to T^2 dependence with increasing doping in the optimally doped to overdoped regime [13, 14]. Furthermore, ρ of underdoped cuprates in the intermediate T range above the temperature of the insulating regime may be fitted by T^α (see the data in Ref. [13, 14]), with α smaller than 1 and decreasing with decreasing x. This is consistent with Eq. (5), where η is expected to be smaller than $\frac{1}{2}$ and decrease with x in the underdoped regime. Since $k_B T \ll E_F^0$ for $T < 300K$, τ_{ee}^{-1} should increase significantly with decreasing η, according to Eq. (6). This means that in the optimally doped to underdoped regime, at room temperature or even above, the electron-electron scattering can still be dominant over other scattering mechanisms, including the electron-phonon scattering. This helps to

explain why the linear T dependence of ρ can be seen up to very high temperature [15]. In addition, a low temperature $\rho \sim T^{\alpha}$ behavior with $0 < \alpha < 2$ has been observed in other narrow band materials, two of the most recent examples are $BaVS_3$ [16] and $La_4Ru_6O_{19}$ [17]. In $BaVS_3$ α can even be tuned by pressure [16]. These are all consistent with Eq. (6) predicted by the p.F. statistics.

We finally come to the calculation of the zero temperature superconducting gap $\Delta(0)$ and the superconducting critical temperature T_c of a p.F. system. A p.F. gas system of course can not superconduct, so we first introduce a BCS-type attractive interaction V. Similar to the assumption in the BCS theory [18], V is supposed to be constant between two partially localized electrons with energies immediately below E_{pF} within a shell of $\hbar\omega_D$ thick, and zero for any other electron pairs. $\hbar\omega_D$ is the energy of phonons, or any other types of bosons that mediate the formation of Cooper pairs. Using the same variational method as in the deduction of the BCS theory [18], and replacing the Fermi statistics by Eqs. (2), (4), and (5), one reaches

$$\begin{aligned} \Delta(0) &\approx 2\hbar\omega_D \, e^{-\eta/g(E_F^0)V}, \\ k_B T_c &\approx \hbar\omega_D [0.783 \, e^{2\eta/g(E_F^0)V} + (\ln\eta)^2]^{-1/2}. \end{aligned} \tag{7}$$

When $\eta = 1$, the BCS expression of $\Delta(0)$ and T_c are recovered. When $\eta = 0$, $\Delta(0) = k_B T_c = 0$. For $g(E_F^0)V = 0.2$, which is a typical weak coupling value, the maximum of T_c (denoted as T_{cm}) is about $0.38\hbar\omega_D$ with a corresponding $\eta \approx 0.135$, as shown in Fig. 2. This is about 50 times of the BCS T_c value with the same $g(E_F^0)V$. With increasing $g(E_F^0)V$, T_{cm} increases, so does the corresponding value of η (denoted as η_m). With $g(E_F^0)V = 1.3$, η_m is about 0.5, the value which we assigned to optimally doped cuprates in the transport properties discussion above. However, Fig. 2 should not be used to compare directly with T_c *vs.* x of superconducting cuprates, since cuprates are d-wave superconductors, and the assumption of V above cannot be applied. Moreover, even for phonon mediating s-wave superconductors a direct comparison is also not possible, because in order to have an η significantly deviating from 1, the electron-phonon interaction will be too strong to allow the assumption of a weak-coupling V. Nevertheless, we believe that no matter what specific form V takes, the basic feature of T_c *vs.* η should remain the same for systems obeying the p.F. statistics. That is, with increasing η, T_c should always first increase from 0, reach a maximum, then decrease monotonically until $\eta = 1$. The reason is that this feature is decided by the p.F.

statistics, not by the specific form of V. In fact, the well known T_c *vs.* n_s/m^* plot produced by Uemura *et al.* [19] is qualitatively similar to the plots in Fig. 2. Note that n_s is the density of superconducting carriers, m^* is the effective mass. Since η is the delocalization degree of p.F. systems, it is thus reasonable to assume that η increases monotonically with n_s/m^*. We also note that the Uemura plot includes many different systems with different superconducting mechanisms, but all of them are narrow band materials [19, 20]. Recently spectacular results have been achieved on C_{60} with injected carriers, and T_c has reached 117 K [21]. In these materials, T_c as a function of injected carrier concentration again shows the same basic feature mentioned above [21]. Because of the narrow band width of C_{60} crystals [20], increasing injected carriers may also have increased the delocalization degree of the carriers in C_{60}, and subsequently caused the change in T_c.

There are still many open questions for the p.F. systems. For example, if the spin degree of freedom cannot be ignored, as in the case of underdoped cuprates which are very close to the antiferromagnetic phase, what kind of change will it bring to the p.F. systems? If the localized electrons become mobile with increasing temperature, how does the partial Fermi energy respond to such a change, especially at high temperature? If electrons are more localized in one direction than another, η might become anisotropic, and how is the anisotropy of η in k-space dependent on the many-body wave function of partially localized electrons? Despite these open questions, this letter nevertheless has demonstrated that materials obeying the p.F. statistics have many properties that are very different from Landau-Fermi liquids, but are consistent with those observed in cuprates and other narrow band materials. We thus believe that the p.F. statistics can not only help to understand why bound electron systems are so different from unbound electron systems [22], it may also provide a starting point to tackle the physics of cuprates and other non-Fermi-liquid metals.

I am very thankful to Dr. D.T. Neilson for his support.

---

* Electronic address: tzhou2@lucent.com

[1] G.H. Wannier, Statistical Physics, John Wiley & Sons, New York, 1966.

[2] C. Kittle, Introduction to Solid State Physics, fourth edition, John Wiley & Sons, New York, 1971.

[3] T. Zhou, Solid State Commun. **115**, 185 (2000).

[4] R. Acharya and P. Narayana Swamy, J. Phys. A: Math. Gen. **27**, 7247 (1994).

[5] A.P. Polychronakos, Phys. Lett. B **365**, 202 (1996).

[6] For reviews of narrow-band materials, see N.F. Mott, Metal-Insulator Transitions, second edition, Taylor & Francis, London, 1990.

[7] The most complete references to the experimental results of cuprates are the proceedings of the last three triannual international conferences on materials and mechanisms of superconductivity: [Physica C **235-240** (1994)]; [Physica C **282-287** (1997)]; and [Physica C **341-348** (2000)].

[8] For a recent review of the cuprates, see J. Orenstein and A.J. Millis, Science **288**, 468 (2000) and K. Kitazawa, Physica C **341**, 19 (2000).

[9] J.W. Loram *et al.*, Physica C **235-240**, 134 (1994); J.W. Loram *et al.*, Physica C **282-287**, 1405 (1997).

[10] C.M. Varma *et al.*, Phys. Rev. Lett. **63**, 1996 (1989).

[11] P.B. Littlewood and C.M. Varma, J. Appl. Phys. **69**, 4979 (1991).

[12] C.M. Varma, Phys. Rev. B **55**, 14554 (1997).

[13] B. Batlogg *et al.*, Physica C **235-240**, 130 (1994).

[14] B. Batlogg, Solid State Commun. **107**, 639 (1998).

[15] S. Martin *et al.*, Phys. Rev. B **41**, 846 (1990); H. Takagi *et al.*, Phys. Rev. Lett. **69**, 2975 (1992).

[16] L. Forró *et al.*, Phys. Rev. Lett. **85**, 1938 (2000).

[17] P. Khalifah *et al.*, Nature **411**, 669 (2001).

[18] J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[19] Y.J. Uemura *et al.*, Phys. Rev. Lett. **66**, 2665 (1991).

[20] Y.J. Uemura *et al.*, Nature **352**, 605 (1991).

[21] J.H. Schön, Ch. Kloc, and B. Batlogg, Nature **408**, 549 (2000); J.H. Schön, Ch. Kloc, and B. Batlogg, Science **293**, 2432 (2001).

[22] P.W. Anderson, Physics Today, February 2000, p. 11.

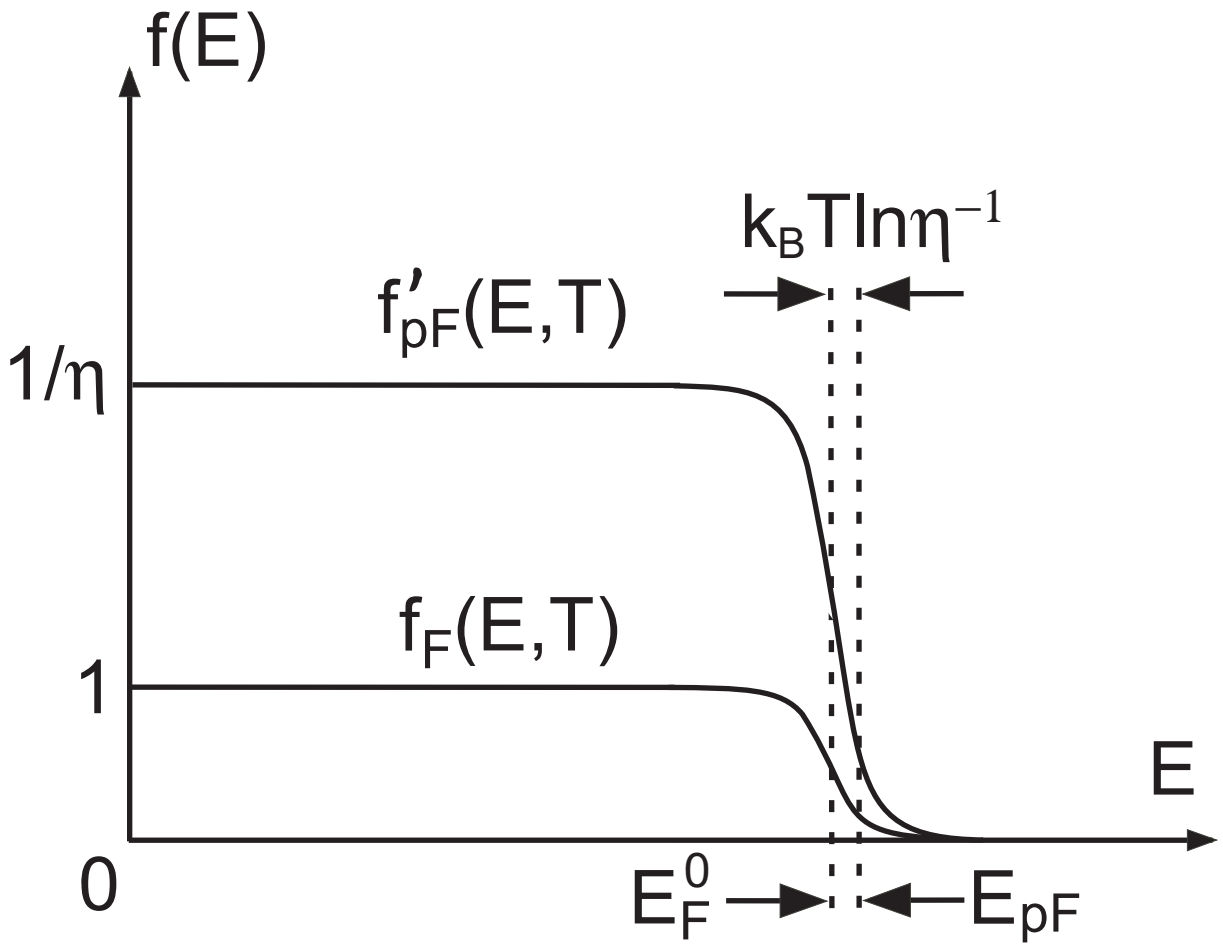

FIG. 1: Schematic illustration of the distribution functions of the Fermi statistics $f_F(E,T)$ and partial Fermi statistics $f'_{pF}(E,T)$ with the same total density of states. The two dashed lines indicate the zero temperature Fermi energy E_F^0 and partial Fermi energy E_{pF}, respectively. Their difference is about $k_B T ln\eta^{-1}$.

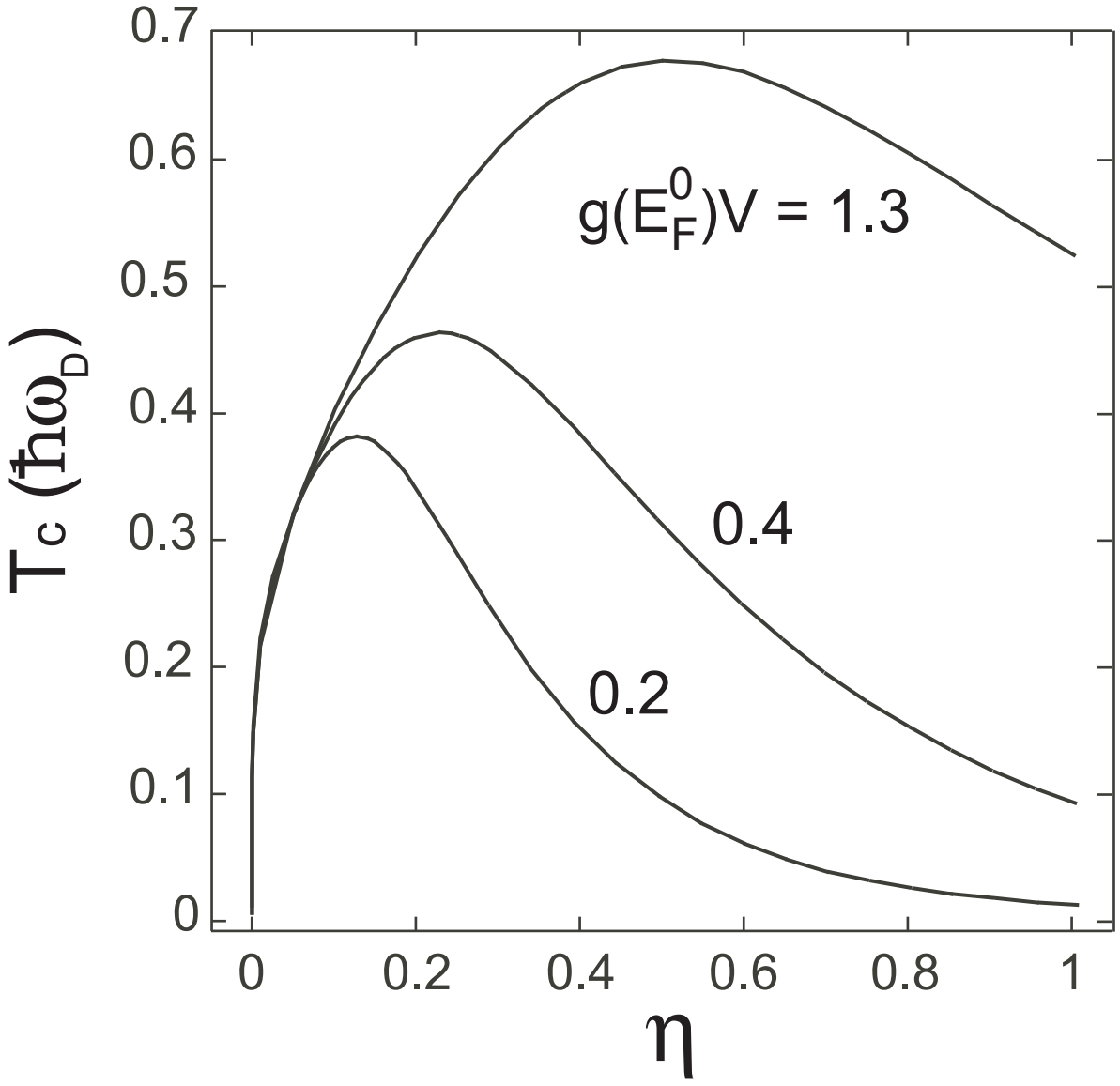

FIG. 2: Calculated T_c of partially localized electron systems as a function of η. The calculations are based on the partial Fermi statistics and a BCS-type interaction between electrons. The unit of T_c is $\hbar\omega_D$. Three different curves correspond to three different values of $g(E_F^0)V$ with $g(E_F^0)V$ = 0.2, 0.4, and 1.3, respectively.